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6-(4-Methylphenyl)-1,3,5-triazine-2,4-diamine–4-methylbenzoic acid (1/1)

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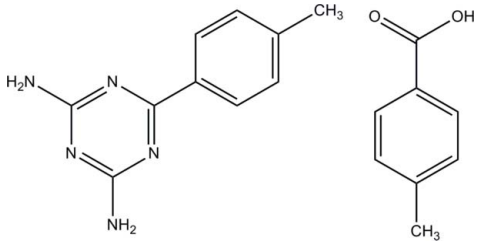
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.006 Å; R factor = 0.055; wR factor = 0.135; data-to-parameter ratio = 7.9.

The 4-methylbenzoic acid molecule of the title adduct, $C_{10}H_{11}N_5\cdot C_8H_8O_2$, is approximately planar with a dihedral angle of 6.3 (2)° between the carboxylic acid group and the benzene ring. In the triazine molecule, the plane of the triazine ring makes a dihedral angle of 29.2 (2)° with that of the adjacent benzene ring. In the crystal, the acid and base molecules are linked *via* N—H···O and O—H···N hydrogen bonds with an $R_2^2(8)$ motif, and the acid–base pairs are further connected *via* N—H···N hydrogen bonds with $R_2^2(8)$ motifs, forming a supramolecular ribbon along [101]. Between the tapes, a weak C—H···π interaction is observed.

Related literature

The background to this study has been described in the preceding paper, see: Thanigaimani *et al.* (2013). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For bond-length data, see: Allen *et al.* (1987). For stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{10}H_{11}N_5\cdot C_8H_8O_2$
M_r = 337.38
Monoclinic, Cc
a = 11.1271 (3) Å
b = 20.9492 (6) Å
c = 7.4189 (2) Å
β = 101.321 (2)°
V = 1695.73 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.40 × 0.40 × 0.20 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.965, T_{max} = 0.982
8715 measured reflections
1932 independent reflections
1811 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.135
S = 1.19
1932 reflections
244 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*2 is the centroid of the C4–C9 ring.

D—H···A	D—H	H···A	D···A	D—H···A
O2—H1*O2*···N2	0.77 (6)	1.92 (6)	2.682 (4)	171 (6)
N4—H1*N4*···O1	0.97 (6)	1.98 (6)	2.936 (5)	169 (6)
N4—H2*N4*···N3^{i}	0.84 (4)	2.26 (4)	3.099 (5)	172 (4)
N5—H1*N5*···N1^{ii}	0.90 (6)	2.11 (6)	3.003 (5)	173 (5)
C10—H10*C*···*Cg*2^{iii}	0.98	2.83	3.723 (6)	152

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $x, -y+1, z-\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5272).

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‡ Thomson Reuters ResearcherID: A-5599-2009.

supplementary materials

Acta Cryst. (2013). E**69**, o970 [doi:10.1107/S1600536813013895]

6-(4-Methylphenyl)-1,3,5-triazine-2,4-diamine–4-methylbenzoic acid (1/1)

Kaliyaperumal Thanigaimani, Suhana Arshad, Ibrahim Abdul Razak, Duraisamy Makeshvaran and Kasthuri Balasubramani

Comment

This work follows on from our previous report on 2,4-diamino-6-(4-methylphenyl)-1,3,5-triazine–benzoic acid (1/1) (Thanigaimani *et al.*, 2013).

The asymmetric unit (Fig. 1) contains one 2,4-diamino-6-(4-methylphenyl)- 1,3,5-triazine molecule and one 4-methylbenzoic acid molecule. The dihedral angle between the triazine ring [N1/C1/N2/C2/N3/C3, maximum deviation = 0.003 (4) Å for atom N1] and the plane formed by the benzoic acid molecule (O1/O2/C11–C18) is 12.04 (19)°. The triazine ring forms a dihedral angle of 29.2 (2)° with the benzene ring (C4–C10). The bond lengths (Allen *et al.*, 1987) and angles are normal.

In the crystal (Fig. 2), the triazine molecules are base-paired with a $R_2^2(8)$ graph-set motifs (Bernstein *et al.*, 1995) on either side *via* N4—H2N4···N3^{ii} and N5—H1N5···N1^{i} hydrogen bonds (symmetry codes in Table 1) and further interact with the carboxyl group of 4-methylbenzoic acid molecules *via* N4—H1N4···O1 and O2—H1O2···N2 hydrogen bonds, forming an $R_2^2(8)$ motif and a supramolecular ribbon along the [101]. In addition, the crystal structure is stabilized by weak C—H···π interactions (Table 1) involving the C4–C9 (centroid C*g*2) ring.

Experimental

Hot methanol solutions (20 ml) of 2,4-diamino-6-(4-methylphenyl)-1,3,5-triazine (50 mg Aldrich) and 4-methylbenzoic acid (34 mg Aldrich) were mixed and warmed over a heating magnetic stirrer hotplate for a few minutes. The resulting solution was allowed to cool slowly at room temperature and crystals of the title compound (I) appeared after a few days.

Refinement

O- and N-bound H atoms were located in a difference Fourier maps. The O-bound H atom was refined freely [refined distance: O2—H1O2 = 0.77 (6) Å], while for the N-bound H atoms the positions were refined with U_{iso}(H) = 1.5U_{eq}(N). [refined distances: N5—H1N5 = 0.90 (6) Å, N5—H2N5 = 0.89 (6) Å, N4—H1N4 = 0.97 (6) Å, N4—H2N4 = 0.849 (11) Å]. A bond-length restraint of N—H = 0.85 (1) Å was also applied for N4—H2N4. The remaining hydrogen atoms were positioned geometrically (C—H = 0.95–0.98 Å) and were refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). A rotating-group model was used for the methyl group. In the final refinement, 1279 Friedel pairs were merged.

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

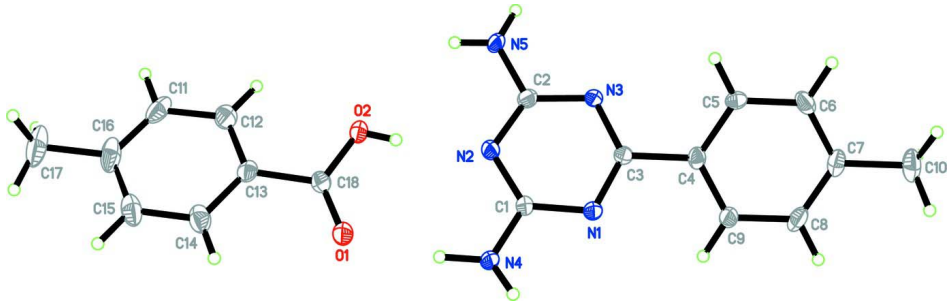

Figure 1

The molecular structure of the title compound with atom labels with 50% probability displacement ellipsoids.

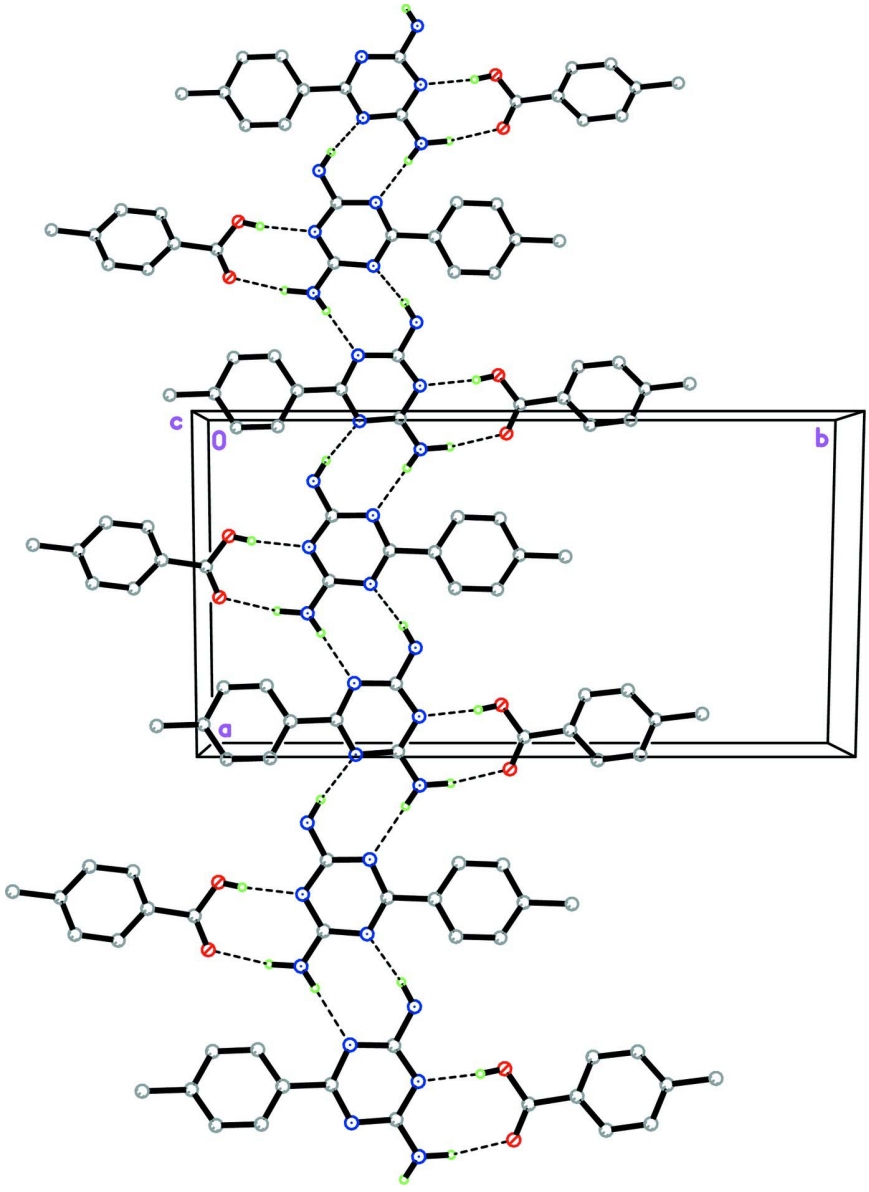

Figure 2

The crystal packing of the title compound. The H atoms not involved in the intermolecular interactions (dashed lines) have been omitted for clarity.

6-(4-Methylphenyl)-1,3,5-triazine-2,4-diamine–4-methylbenzoic acid (1/1)

Crystal data

$C_{10}H_{11}N_5 \cdot C_8H_8O_2$
$M_r = 337.38$
Monoclinic, *Cc*
Hall symbol: C -2yc
$a = 11.1271$ (3) Å
$b = 20.9492$ (6) Å
$c = 7.4189$ (2) Å
$\beta = 101.321$ (2)°
$V = 1695.73$ (8) Å^3
$Z = 4$
$F(000) = 712$
$D_x = 1.322$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6815 reflections
$\theta = 3.2$–33.7°
$\mu = 0.09$ mm^{-1}

T = 100 K
Plate, colourless

0.40 × 0.40 × 0.20 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.965, T_{max} = 0.982

8715 measured reflections
1932 independent reflections
1811 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 27.5°, θ_{min} = 1.9°
h = −14→14
k = −27→27
l = −9→7

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.135
S = 1.19
1932 reflections
244 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0311P)^2 + 4.4301P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
N1	0.4994 (3)	0.25996 (17)	0.3556 (5)	0.0165 (8)
N2	0.3884 (4)	0.16295 (15)	0.2802 (6)	0.0170 (7)
N3	0.2919 (3)	0.26326 (16)	0.1933 (6)	0.0164 (7)
N4	0.5874 (3)	0.16186 (18)	0.4348 (5)	0.0200 (8)
H1N4	0.581 (5)	0.116 (3)	0.447 (8)	0.030*
H2N4	0.646 (3)	0.183 (2)	0.496 (7)	0.030*
N5	0.1876 (3)	0.16862 (19)	0.1268 (6)	0.0235 (9)
H1N5	0.126 (5)	0.188 (3)	0.049 (9)	0.035*
H2N5	0.188 (5)	0.126 (3)	0.120 (8)	0.035*
C1	0.4899 (4)	0.19523 (19)	0.3563 (6)	0.0156 (8)
C2	0.2928 (4)	0.19889 (19)	0.2015 (6)	0.0169 (8)
C3	0.3982 (4)	0.29042 (16)	0.2738 (7)	0.0150 (7)

C4	0.4034 (4)	0.36131 (17)	0.2713 (7)	0.0166 (8)
C5	0.2976 (4)	0.3973 (2)	0.2713 (6)	0.0189 (9)
H5A	0.2217	0.3762	0.2690	0.023*
C6	0.3023 (4)	0.4632 (2)	0.2746 (7)	0.0228 (10)
H6A	0.2296	0.4870	0.2744	0.027*
C7	0.4126 (4)	0.49501 (18)	0.2781 (7)	0.0216 (9)
C8	0.5170 (4)	0.4596 (2)	0.2779 (7)	0.0236 (10)
H8A	0.5926	0.4809	0.2798	0.028*
C9	0.5136 (4)	0.39311 (19)	0.2749 (6)	0.0187 (9)
H9A	0.5865	0.3695	0.2753	0.022*
C10	0.4170 (5)	0.5672 (2)	0.2789 (8)	0.0306 (11)
H10A	0.4988	0.5814	0.3396	0.046*
H10B	0.3558	0.5838	0.3455	0.046*
H10C	0.3991	0.5830	0.1521	0.046*
O1	0.5390 (3)	0.02412 (14)	0.4355 (5)	0.0245 (7)
O2	0.3551 (3)	0.03627 (15)	0.2514 (5)	0.0248 (7)
C11	0.3135 (5)	−0.1599 (2)	0.1798 (7)	0.0298 (12)
H11A	0.2450	−0.1770	0.0970	0.036*
C12	0.3269 (4)	−0.0939 (2)	0.1967 (7)	0.0253 (10)
H12A	0.2683	−0.0662	0.1258	0.030*
C13	0.4271 (4)	−0.0689 (2)	0.3187 (6)	0.0201 (10)
C14	0.5126 (5)	−0.1101 (2)	0.4226 (7)	0.0268 (10)
H14A	0.5807	−0.0934	0.5069	0.032*
C15	0.4970 (5)	−0.1754 (2)	0.4014 (7)	0.0305 (12)
H15A	0.5557	−0.2033	0.4711	0.037*
C16	0.3977 (6)	−0.20104 (19)	0.2808 (10)	0.0338 (12)
C17	0.3816 (7)	−0.2731 (2)	0.2623 (12)	0.0459 (16)
H17A	0.3450	−0.2838	0.1348	0.069*
H17B	0.3278	−0.2879	0.3437	0.069*
H17C	0.4617	−0.2939	0.2967	0.069*
C18	0.4468 (4)	0.0016 (2)	0.3420 (6)	0.0202 (9)
H1O2	0.370 (6)	0.072 (3)	0.253 (9)	0.038 (16)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0140 (17)	0.0145 (17)	0.0190 (18)	−0.0002 (14)	−0.0018 (15)	−0.0001 (15)
N2	0.0159 (16)	0.0136 (14)	0.0195 (15)	0.0007 (15)	−0.0012 (13)	−0.0001 (17)
N3	0.0125 (15)	0.0127 (17)	0.0224 (18)	0.0006 (14)	−0.0002 (14)	0.0021 (15)
N4	0.0155 (17)	0.0140 (17)	0.027 (2)	−0.0007 (14)	−0.0055 (15)	−0.0017 (15)
N5	0.0146 (18)	0.0144 (19)	0.037 (2)	−0.0030 (14)	−0.0063 (17)	0.0027 (16)
C1	0.0154 (18)	0.0128 (18)	0.0183 (19)	0.0004 (16)	0.0024 (16)	0.0000 (17)
C2	0.0151 (18)	0.017 (2)	0.018 (2)	−0.0021 (17)	0.0015 (16)	0.0000 (18)
C3	0.0138 (17)	0.0147 (16)	0.0168 (17)	0.0002 (17)	0.0041 (14)	−0.0008 (19)
C4	0.0211 (19)	0.0130 (16)	0.0141 (18)	0.0003 (18)	−0.0009 (15)	−0.0020 (19)
C5	0.0129 (19)	0.020 (2)	0.021 (2)	−0.0008 (16)	−0.0049 (16)	−0.0015 (17)
C6	0.022 (2)	0.019 (2)	0.024 (2)	0.0083 (18)	−0.0040 (18)	−0.0040 (18)
C7	0.032 (2)	0.0132 (17)	0.0169 (18)	−0.0022 (19)	−0.0026 (18)	0.000 (2)
C8	0.025 (2)	0.017 (2)	0.027 (2)	−0.0084 (17)	0.0001 (19)	0.0010 (18)
C9	0.018 (2)	0.0148 (19)	0.021 (2)	−0.0005 (16)	−0.0018 (17)	−0.0002 (17)

C10	0.047 (3)	0.0130 (18)	0.030 (2)	0.002 (2)	0.003 (2)	0.001 (2)
O1	0.0219 (16)	0.0158 (13)	0.0323 (18)	−0.0005 (13)	−0.0035 (13)	0.0004 (14)
O2	0.0205 (15)	0.0135 (14)	0.037 (2)	−0.0021 (12)	−0.0022 (14)	0.0019 (14)
C11	0.031 (3)	0.024 (2)	0.039 (3)	−0.013 (2)	0.019 (2)	−0.015 (2)
C12	0.025 (2)	0.020 (2)	0.034 (3)	0.0007 (18)	0.014 (2)	−0.007 (2)
C13	0.019 (2)	0.0170 (19)	0.028 (3)	−0.0016 (16)	0.0145 (19)	−0.0006 (17)
C14	0.032 (3)	0.019 (2)	0.033 (3)	0.0043 (19)	0.015 (2)	0.003 (2)
C15	0.041 (3)	0.020 (2)	0.036 (3)	0.008 (2)	0.020 (2)	0.009 (2)
C16	0.052 (3)	0.0146 (19)	0.045 (3)	−0.001 (2)	0.034 (2)	−0.005 (3)
C17	0.074 (4)	0.017 (2)	0.058 (4)	−0.008 (3)	0.041 (3)	−0.005 (3)
C18	0.019 (2)	0.0158 (19)	0.026 (2)	0.0017 (17)	0.0062 (18)	−0.002 (2)

Geometric parameters (Å, º)

N1—C3	1.333 (5)	C9—H9A	0.9500
N1—C1	1.360 (5)	C10—H10A	0.9800
N2—C2	1.340 (5)	C10—H10B	0.9800
N2—C1	1.342 (6)	C10—H10C	0.9800
N3—C3	1.342 (5)	O1—C18	1.215 (5)
N3—C2	1.350 (5)	O2—C18	1.324 (5)
N4—C1	1.326 (5)	O2—H1O2	0.77 (6)
N4—H1N4	0.97 (6)	C11—C16	1.380 (8)
N4—H2N4	0.849 (11)	C11—C12	1.395 (6)
N5—C2	1.351 (5)	C11—H11A	0.9500
N5—H1N5	0.90 (6)	C12—C13	1.393 (6)
N5—H2N5	0.89 (6)	C12—H12A	0.9500
C3—C4	1.487 (5)	C13—C14	1.398 (6)
C4—C9	1.390 (6)	C13—C18	1.498 (6)
C4—C5	1.398 (6)	C14—C15	1.384 (6)
C5—C6	1.382 (6)	C14—H14A	0.9500
C5—H5A	0.9500	C15—C16	1.386 (8)
C6—C7	1.392 (7)	C15—H15A	0.9500
C6—H6A	0.9500	C16—C17	1.523 (6)
C7—C8	1.378 (6)	C17—H17A	0.9800
C7—C10	1.512 (5)	C17—H17B	0.9800
C8—C9	1.394 (6)	C17—H17C	0.9800
C8—H8A	0.9500		

C3—N1—C1	114.8 (3)	C8—C9—H9A	120.0
C2—N2—C1	115.5 (3)	C7—C10—H10A	109.5
C3—N3—C2	113.9 (3)	C7—C10—H10B	109.5
C1—N4—H1N4	120 (3)	H10A—C10—H10B	109.5
C1—N4—H2N4	116 (4)	C7—C10—H10C	109.5
H1N4—N4—H2N4	122 (5)	H10A—C10—H10C	109.5
C2—N5—H1N5	123 (4)	H10B—C10—H10C	109.5
C2—N5—H2N5	119 (4)	C18—O2—H1O2	113 (5)
H1N5—N5—H2N5	115 (5)	C16—C11—C12	121.4 (5)
N4—C1—N2	117.9 (4)	C16—C11—H11A	119.3
N4—C1—N1	118.0 (4)	C12—C11—H11A	119.3
N2—C1—N1	124.1 (4)	C13—C12—C11	119.2 (5)

N2—C2—N3	125.4 (4)	C13—C12—H12A	120.4
N2—C2—N5	117.7 (4)	C11—C12—H12A	120.4
N3—C2—N5	116.9 (4)	C12—C13—C14	119.9 (4)
N1—C3—N3	126.3 (3)	C12—C13—C18	121.7 (4)
N1—C3—C4	116.9 (4)	C14—C13—C18	118.5 (4)
N3—C3—C4	116.8 (3)	C15—C14—C13	119.4 (5)
C9—C4—C5	118.8 (3)	C15—C14—H14A	120.3
C9—C4—C3	121.0 (4)	C13—C14—H14A	120.3
C5—C4—C3	120.2 (4)	C14—C15—C16	121.5 (5)
C6—C5—C4	120.6 (4)	C14—C15—H15A	119.2
C6—C5—H5A	119.7	C16—C15—H15A	119.2
C4—C5—H5A	119.7	C11—C16—C15	118.6 (4)
C5—C6—C7	120.6 (4)	C11—C16—C17	121.0 (6)
C5—C6—H6A	119.7	C15—C16—C17	120.5 (6)
C7—C6—H6A	119.7	C16—C17—H17A	109.5
C8—C7—C6	118.9 (4)	C16—C17—H17B	109.5
C8—C7—C10	120.7 (4)	H17A—C17—H17B	109.5
C6—C7—C10	120.4 (4)	C16—C17—H17C	109.5
C7—C8—C9	121.2 (4)	H17A—C17—H17C	109.5
C7—C8—H8A	119.4	H17B—C17—H17C	109.5
C9—C8—H8A	119.4	O1—C18—O2	123.8 (4)
C4—C9—C8	120.0 (4)	O1—C18—C13	122.5 (4)
C4—C9—H9A	120.0	O2—C18—C13	113.7 (4)

C2—N2—C1—N4	−179.5 (4)	C5—C6—C7—C10	179.1 (5)
C2—N2—C1—N1	−0.5 (7)	C6—C7—C8—C9	−0.2 (8)
C3—N1—C1—N4	179.7 (4)	C10—C7—C8—C9	−179.2 (4)
C3—N1—C1—N2	0.7 (7)	C5—C4—C9—C8	−0.2 (7)
C1—N2—C2—N3	0.3 (7)	C3—C4—C9—C8	−178.1 (4)
C1—N2—C2—N5	−178.5 (4)	C7—C8—C9—C4	0.3 (7)
C3—N3—C2—N2	−0.3 (7)	C16—C11—C12—C13	−0.2 (7)
C3—N3—C2—N5	178.5 (4)	C11—C12—C13—C14	−0.1 (7)
C1—N1—C3—N3	−0.7 (8)	C11—C12—C13—C18	179.6 (4)
C1—N1—C3—C4	179.3 (4)	C12—C13—C14—C15	0.6 (7)
C2—N3—C3—N1	0.5 (8)	C18—C13—C14—C15	−179.2 (5)
C2—N3—C3—C4	−179.5 (4)	C13—C14—C15—C16	−0.7 (8)
N1—C3—C4—C9	28.0 (7)	C12—C11—C16—C15	0.2 (8)
N3—C3—C4—C9	−152.0 (5)	C12—C11—C16—C17	179.5 (5)
N1—C3—C4—C5	−149.9 (5)	C14—C15—C16—C11	0.3 (9)
N3—C3—C4—C5	30.1 (7)	C14—C15—C16—C17	−179.0 (6)
C9—C4—C5—C6	0.1 (7)	C12—C13—C18—O1	−173.4 (4)
C3—C4—C5—C6	178.0 (4)	C14—C13—C18—O1	6.4 (7)
C4—C5—C6—C7	−0.1 (7)	C12—C13—C18—O2	6.4 (6)
C5—C6—C7—C8	0.1 (8)	C14—C13—C18—O2	−173.8 (4)

Hydrogen-bond geometry (Å, º)

*Cg*2 is the centroid of the C4–C9 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1*O*2···N2	0.77 (6)	1.92 (6)	2.682 (4)	171 (6)
N4—H1*N*4···O1	0.97 (6)	1.98 (6)	2.936 (5)	169 (6)
N4—H2*N*4···N3^{i}	0.84 (4)	2.26 (4)	3.099 (5)	172 (4)
N5—H1*N*5···N1^{ii}	0.90 (6)	2.11 (6)	3.003 (5)	173 (5)
C10—H10*C*···*Cg*2^{iii}	0.98	2.83	3.723 (6)	152

Symmetry codes: (i) *x*+1/2, −*y*+1/2, *z*+1/2; (ii) *x*−1/2, −*y*+1/2, *z*−1/2; (iii) *x*, −*y*+1, *z*−1/2.